Reduced-order model for the BGK equation based on POD and optimal transport

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Contribution

We present a model describing a gas flow in both hydrodynamic and rarefied regimes. Since the computational cost of the Bhatnagar-Gross-Krook (BGK) equation can be prohibitive, a reduced-order approximation is developed, leading to fast and accurate simulations.

BGK equation

The dynamics of the gas flow is described by the **BGK equation**:

$$\frac{\partial f}{\partial t}(\mathbf{x},\xi,t) + \xi \cdot \nabla_{\mathbf{x}} f(\mathbf{x},\xi,t) = \frac{M_f(\mathbf{x},\xi,t) - f(\mathbf{x},\xi,t)}{\tau(\mathbf{x},t)} \qquad (1)$$

where f is the density distribution function representing the density of gas particles at point $\mathbf{x} \in \mathbb{R}^3$, velocity $\xi \in \mathbb{R}^3$ and time $t \in \mathbb{R}$. The Maxwellian distribution function M_f is in dimensionless form

$$M_f(\mathbf{x},\xi,t) = \frac{\rho(\mathbf{x},t)}{(2\pi T(\mathbf{x},t))^{\frac{3}{2}}} \exp\left(-\frac{\|\xi - U(\mathbf{x},t)\|^2}{2T(\mathbf{x},t)}\right)$$

where $\rho \in \mathbb{R}$ is the density, $U \in \mathbb{R}^3$ is the macroscopic velocity, $T \in \mathbb{R}$ is the temperature and $E \in \mathbb{R}$ is the total energy of the gas.

Reduced-order approximation

The distribution functions are approximated by

$$\widetilde{f}(\mathbf{x},\xi,t) = \sum_{n=1}^{N_{pod}} a_n^f(\mathbf{x},t)\Phi_n(\xi)$$

and

$$\widetilde{M}_f(\mathbf{x},\xi,t) = \sum_{n=1}^{N_{pod}} a_n^M(\mathbf{x},t)\Phi_n(\xi)$$

where the basis functions Φ_n are built offline by **Proper Orthogonal Decomposition** (POD) and the coefficients a_n are computed online by the **Galerkin method**.

References

[1] P. L. Bhatnagar, E. P. Gross and M. Krook. *A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems.* Physical Review, 1954.

[2] F. Bernard. *Efficient asymptotic preserving schemes for BGK and ES-BGK models on cartesian grids.* PhD thesis, 2015.

[3] F. Bernard, A. Iollo and S. Riffaud. *Reduced-order model for the BGK equation based on POD and optimal transport.* Journal of Computational Physics, 2018.

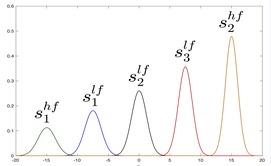
Offline phase

In the offline phase, the BGK equation (1) is sampled to collect information on the distribution functions that we want to approximate. High-fidelity simulations provide snapshots of both the density distribution function and of the Maxwellian distribution function:

$$S^{\text{hf}} = \left\{f(\mathbf{x}_i,\xi,t_k)\right\}_{\substack{1\le i\le N_{\mathbf{x}}\\ 1\le k\le N_t}} \bigcup \left\{M_f(\mathbf{x}_i,\xi,t_k)\right\}_{\substack{1\le i\le N_{\mathbf{x}}\\ 1\le k\le N_t}}$$

Then, **optimal transport** provides additional low-fidelity snapshots by interpolating the snapshots of S^{hf} to complete the sampling:

$$S = S^{\text{hf}} \cup S^{\text{lf}}$$



Finally, the basis functions Φ_n are built by POD to have the best approximation in the least squares sense of the snapshots $s_l \in S$:

$$\begin{cases} \underset{\Phi_1(\xi)\dots\Phi_{N_{pod}}(\xi)}{\text{minimize}} & \displaystyle\sum_{l=1}^{N_{snaps}} \int_{\mathbb{R}^3} \left(s_l(\xi) - \mathcal{P}[s_l](\xi)\right)^2 \mathrm{d}\xi \\ \text{subject to} & \displaystyle\int_{\mathbb{R}^3} \Phi_n(\xi)\Phi_m(\xi)\,\mathrm{d}\xi = \delta_{n,m} \end{cases}$$

where $\mathcal{P}[s_l]$ is the projection of s_l onto the subspace spanned by the basis functions Φ_n $\left(\text{i.e. } \mathcal{P}[s_l](\xi) = \sum_{n=1}^{N_{pod}} \int_{\mathbb{R}^3} s_l(\xi')\Phi_n(\xi')\,\mathrm{d}\xi'\ \Phi_n(\xi)\right)$.

Online phase

During the online phase, the offline knowledge is used to compute approximations of the distribution functions at low cost. In the Galerkin method, the BGK equation (1) is projected onto the basis functions Φ_n, leading to an **hyperbolic system** of partial differential equations:

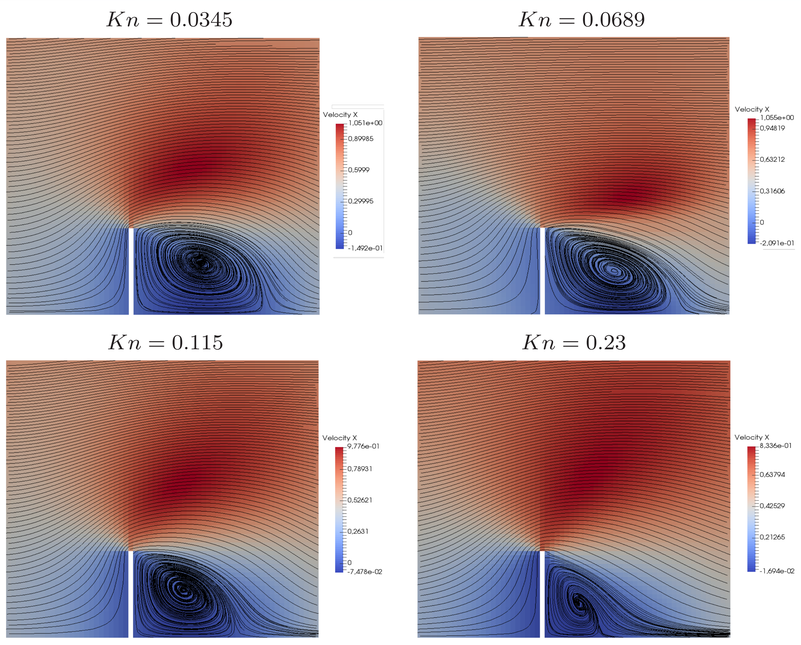
$$\frac{\partial a^f}{\partial t}(\mathbf{x},t) + A\frac{\partial a^f}{\partial x}(\mathbf{x},t) + \mathring{A}\frac{\partial a^f}{\partial y}(\mathbf{x},t) + \mathring{A}\frac{\partial a^f}{\partial z}(\mathbf{x},t) = \frac{a^M(\mathbf{x},t) - a^f(\mathbf{x},t)}{\tau(\mathbf{x},t)}$$

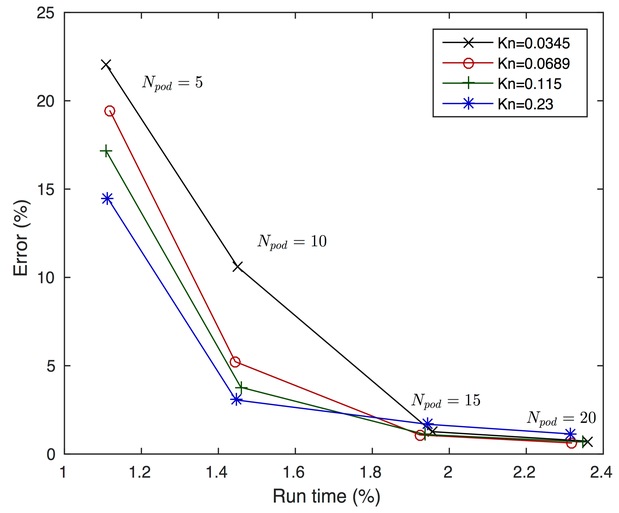
where $a = (a_1, a_2, \dots, a_{N_{pod}})^T$, $A_{n,m} = \int_{\mathbb{R}^3} \xi_u \Phi_n(\xi)\Phi_m(\xi)\,\mathrm{d}\xi$, $\mathring{A}_{n,m} = \int_{\mathbb{R}^3} \xi_v \Phi_n(\xi)\Phi_m(\xi)\,\mathrm{d}\xi$ and $\mathring{A}_{n,m} = \int_{\mathbb{R}^3} \xi_w \Phi_n(\xi)\Phi_m(\xi)\,\mathrm{d}\xi$. These equations are decoupled by linear changes of variables and are solved by an **IMEX Runge-Kutta** scheme in time and a **finite volume** scheme in space. To improve the accuracy of the model, the coefficients a_n^M are computed by constrained projection:

$$\begin{cases} \underset{a_1^M(\mathbf{x},t)\dots a_{N_{pod}}^M(\mathbf{x},t)}{\text{minimize}} & \displaystyle\int_{\mathbb{R}^3} \left(M_f(\mathbf{x},\xi,t) - \widetilde{M}_f(\mathbf{x},\xi,t)\right)^2 \mathrm{d}\xi \\ \text{subject to} & \displaystyle\int_{\mathbb{R}^3} \widetilde{M}_f(\mathbf{x},\xi,t) \begin{pmatrix} 1 \\ \xi \\ \frac{\|\xi\|^2}{2} \end{pmatrix} \mathrm{d}\xi = \begin{pmatrix} \rho(\mathbf{x},t) \\ \rho(\mathbf{x},t)U(\mathbf{x},t) \\ E(\mathbf{x},t) \end{pmatrix} \end{cases}$$

in order **to conserve mass, momentum and total energy** of the gas.

Results





In average with $N_{pod} = 20$ basis functions, **the approximation error is less than 1% and the run time is divided by approximately 45** with respect to the high-fidelity simulations.